Towards protein structure solution de novo from powder MAD data

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We seek to develop a new method of de novo structure solution from powder diffraction data, using f ' difference Fourier techniques akin to the so-called 'MAD method'.
This is so as to make accessible to structure determination those samples only producible in powder form but whose structures are needed in structural chemistry and/or structural biology research. A first paper of concept with a test sample (nickel sulphate hexahydrate) has been published using data from SRS 2.3[1]. By collection of data close to the absorption edge, and at a wavelength away from the absorption edge, and after appropriate scaling, it proved possible to compute precise enough differences in intensity arising from the difference of the Ni f ' alone. Structure solution then involved the determination of the site of this Ni atom by conventional structure solving methods, namely the Patterson method, with location of the remaining atoms by difference Fourier techniques. We have also conducted theoretical based SIR phasing evaluations based on Δf ' signals alone. Hence, with experimental MAD data from a single crystal data of a brominated oligonucleotide, we obtained successful phasing from f ' dip to ref wavelength data set dispersive differences alone (ie without f " differences). We have most recently recorded two wavelength f ' dip and reference wavelength data for the bromine K edge for bromine soaked Hen Egg White Lysozyme (HEWL) on SRS 9.1. The Le Bail fit is good (figure 1 is for the f ' dip HEWL data). Our progress will be reported and plans to extend the work to Ledges.

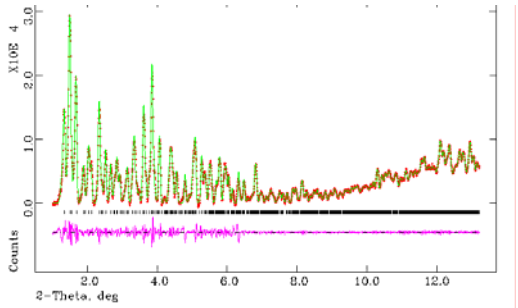

Figure 1 Le Bail fit of the f ' dip SRS 9.1 HEWL powder data.

References

[1] '**Ab initio** structure determination using dispersive differences from multiple-wavelength synchrotron-radiation powder diffraction data' JR Helliwell, M Helliwell & R H Jones, Acta Cryst. (2005). A61, 568-574.